Boltzmann theory of magnetoresistance due to a spin spiral

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We studied the magnetoresistance due to a spin spiral by solving the Boltzmann equation. The scattering rates of conduction electrons are calculated by using the non-perturbative wave function of the conduction electrons and the non-equilibrium distribution function is obtained by numerically solving the Boltzmann equation. These enable us to calculate the resistivity of a sufficiently thin spin spiral. A magnetoresistance ratio of more than 50 % is predicted for a spin spiral with high spin polarization ($\geq$0.8) and a small period (about 1-2 nm).

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There is great interest currently in spin-dependent transport phenomena in magnetic domain walls such as the magnetoresistance (MR) effect[1,2,3,4,5] and spin-transfer torque-driven magnetization dynamics[6,7,8,9] because of the potential application of these phenomena to spin-electronics devices such as spin-motive-force memory[10] and racetrack memory[11]. In these devices, higher magnetoresistance due to a thin domain wall is desirable for high-density magnetic recording.

In 1997, Levy and Zhang[4] studied the resistivity due to domain wall scattering by using the same Hamiltonian that was used to explain the giant magnetoresistance effect. They found that the magnetoresistance ratio is proportional to $1/d^2$, where d is the thickness of the domain wall, and showed that the magnetoresistance ratio is between 2% and 11%, which is consistent with the experimental results (5%) of Ref.[1] where the thickness of the domain wall is about 15 nm.

However, the theory of Levy and Zhang[4] cannot be applied to a sufficiently thin domain wall for two reasons. First, the scattering rates of the conduction electrons are calculated by using the perturbative wave function, which is up to the first order of the dimensionless parameter ξ. The parameter $\xi = l_J/d$ characterizes the non-adiabaticity of the spins of the conduction electrons with respect to the localized spins, where $l_J = \pi\hbar v_{\rm F}/(4J)$ is the electrons' traveling length during the precession of their spins around the sd-exchange field J. For a domain wall with $\xi \geq 1$, the theory cannot estimate the amount of the non-adiabaticity correctly, and thus cannot be applied. Second, since Levy and Zhang applied the diffusion approximation to the Boltzmann equation, their theory cannot be applied to the domain wall in the ballistic region $d \leq l_{\rm mfp}$, where $l_{\rm mfp}$ is the mean free path. For conventional ferromagnetic metals such as Fe, Co, Ni, and their alloys, both l_J and $l_{\rm mfp}$ are on the order of a few nm[12].

The thickness of a domain wall is determined by the competition of the exchange coupling between the localized magnetizations and the magnetic anisotropy, and is usually on the order of 50 nm for conventional ferromagnetic metals. Recently, however, the production of the domain wall of $Co_{50}Fe_{50}$, with a thickness of about 2.5 nm, was achieved by trapping the domain wall in a current-confined-path (CCP) geometry[13], and a magnetoresistance ratio of about 7% -10% was observed. Many studies have examined to understand the physical properties of the CCP structure and applied that structure to magnetic devices[14,15]. To investigate the transport properties of such a thin magnetic structure, in which the system size d is comparable to or less than l_J and $l_{\rm mfp}$, i.e., a few nm, it is important to develop the theory of Levy and Zhang to take into account the amount of the non-adiabaticity correctly and to describe the transport without the diffusion approximation.

In this paper, we study the dependence of the magnetoresistance ratio of a spin spiral on its period (thickness) d by solving the Boltzmann equation. We extend the theory of Levy and Zhang[4] by using the non-perturbative wave function of the conduction electrons in the calculation of the scattering rates and by solving the Boltzmann equation of the non-equilibrium distribution function numerically. These enable us to investigate the resistivity due to a spin spiral with $d < l_J, l_{\rm mfp}$. We find that the MR ratio is more than 50% for a spin spiral with high spin polarization ($\beta \geq 0.8$) and a small period ($d \simeq 1-2$nm). We also find that in the diffusive region, $d \geq l_J, l_{\rm mfp}$, the MR ratio is proportional to $1/d^2$, while in the ballistic region, $d \leq l_J, l_{\rm mfp}$, the MR ratio increases with decreasing d more slowly than it does in the diffusive region.

We consider electron transport in a one-dimensional spin spiral that lies over $-d/2 \leq x \leq d/2$, where d is the period of the π-rotation of the localized spins. We assume that the spin-dependent transport of the conduction electrons is described by the following Hamiltonian:

$$\hat{H}_0 = -\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 - J\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{S}}(\mathbf{r}), \tag{1}$$

where J is the sd-exchange coupling constant between the conduction (s-like) electrons and localized (d-like) spin, $\hat{\boldsymbol{\sigma}}$ is the vector of the Pauli matrices and $\hat{\mathbf{S}} = (0, -\sin\theta, \cos\theta)$ is the unit vector along the direction of the localized spin. The angle θ is given by $\theta(x) = (\pi/d)(x + d/2)$. On the other hand, the spin-dependent

impurity scattering is described by[4]

$$\hat{V}=\sum_i \left[v-j\hat{\boldsymbol{\sigma}}\cdot\hat{\mathbf{S}}(\mathbf{r})\right]\delta(\mathbf{r}-\mathbf{R}_i), \tag{2}$$

where $\mathbf{R}_i$ is the position of the impurity, and v and j are the spin-independent and spin-dependent scattering potentials, respectively. The dependence of the transport properties on the direction of the electrons' spin arises from either the exchange energy J or the spin-dependent scattering potential j, i.e., the spin dependence of the number of the conduction electrons at Fermi level is due to J, and the spin dependence of the scattering rate is due to j.

The resistivity of the spin spiral is calculated by solving the Boltzmann equation of the non-equilibrium distribution function $f^s(\mathbf{k})$ given by

$$\begin{aligned}-ev_x^s E\delta(\varepsilon_{\mathrm{F}}-\varepsilon(\mathbf{k},s)) =&\int\frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}W_{\mathbf{k}\mathbf{k}'}^{ss}[f^s(\mathbf{k})-f^s(\mathbf{k}')]\\ &+\int\frac{\mathrm{d}^3\mathbf{k}'}{(2\pi)^3}W_{\mathbf{k}\mathbf{k}'}^{s-s}[f^s(\mathbf{k})-f^{-s}(\mathbf{k}')],\end{aligned} \tag{3}$$

where $W_{\mathbf{k}\mathbf{k}'}^{ss'}$ is the scattering rate of the conduction electrons from the state $(\mathbf{k},s)$ to the state $(\mathbf{k}',s')$, ε_{F} is the Fermi energy and E is the strength of the applied electric field. The index $s,s'=\pm$ denotes the eigenstate of $\hat{H}_0$ in spin space, which is given by[16]

$$\Psi_{\pm}(\mathbf{r})=\mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}}\exp\left[-\mathrm{i}\frac{\theta(x)}{2}\hat{\sigma}_x\right]\exp\left[-\mathrm{i}\frac{\phi(k_x)}{2}\hat{\sigma}_y\right]\eta_{\pm}\ . \tag{4}$$

Here the angle $\phi(k_x)$ and the spinor $\eta_{\pm}$ are given by

$$\frac{\phi(k_x)}{2}=\arctan\left[\frac{k_x\theta'}{k_J^2+\sqrt{(k_x\theta')^2+k_J^4}}\right], \tag{5}$$

$$\eta_+=\begin{pmatrix}1\\0\end{pmatrix}, \qquad \eta_-=\begin{pmatrix}0\\1\end{pmatrix}, \tag{6}$$

where $\theta'=\mathrm{d}\theta/\mathrm{d}x=\pi/d$ and $k_J=\sqrt{2mJ}/\hbar$, respectively. The factor $\tan(\phi/2)$ characterizes the non-adiabaticity of the spins of the conduction electrons with respect to the localized spins, and is the most important parameter in our calculations. It should be noted that this factor is always less than unity for any period d and momentum k_x. For a sufficiently large period d, $\tan(\phi/2)\to(k_x\theta')/(2k_J^2)=(k_x/k_{\mathrm{F}})\xi$, and the wave function (4) is reduced to the wave function calculated by Levy and Zhang[4]. On the other hand, for a small period d where $\xi=l_J/d$ is comparable to or larger than unity, the wave function (4) does not equal the wave function given in Ref.[4]. The eigenvalue of $\hat{H}_0$ is given by

$$\varepsilon(\mathbf{k},s)=\frac{\hbar^2}{2m}\left[k^2+\left(\frac{\theta'}{2}\right)^2-s\sqrt{(k_x\theta')^2+k_J^4}\right]. \tag{7}$$

The velocity v_x^s is given by $v_x^s=\partial\varepsilon(\mathbf{k},s)/\partial p_x$. The scattering rates are calculated by using the Fermi golden rule with the Born approximation,

$$W_{\mathbf{k}\mathbf{k}'}^{ss'}=\frac{2\pi}{\hbar}|V_{\mathbf{k}\mathbf{k}'}^{ss'}|^2\delta(\varepsilon(\mathbf{k},s)-\varepsilon(\mathbf{k}',s')), \tag{8}$$

where the matrix elements of the sattering potential (2) are calculated by using the wave function (4) and are given by

$$|V_{\mathbf{k}\mathbf{k}'}^{ss}|^2=c_{\mathrm{i}}\left[(v-sj)\cos\frac{\phi}{2}\cos\frac{\phi'}{2}+(v+sj)\sin\frac{\phi}{2}\sin\frac{\phi'}{2}\right]^2, \tag{9}$$

$$|V_{\mathbf{k}\mathbf{k}'}^{s-s}|^2=c_{\mathrm{i}}\left[(-sv+j)\cos\frac{\phi}{2}\sin\frac{\phi'}{2}+(sv+j)\sin\frac{\phi}{2}\cos\frac{\phi'}{2}\right]^2, \tag{10}$$

respectively, where c_{i} is the impurity concentration. Here, for simplicity, we denote $\phi(k_x)$ and $\phi(k_x')$ as ϕ and ϕ', respectively. In the limit of $d\to\infty$, the conduction electrons change the direction of their spins adiabatically, and thus, $\tan(\phi/2)\to 0$ for any momentum k_x. In this limit, the spin-flip scattering rate is zero, i.e., $V_{\mathbf{k}\mathbf{k}'}^{s-s}=0$, and the spin-conserved scattering rate, $W_{\mathbf{k}\mathbf{k}'}^{ss}\propto|V_{\mathbf{k}\mathbf{k}'}^{ss}|^2$, is independent of the momentum k_x. On the other hand, in the limit of $d\to 0$, $\tan(\phi/2)\to 1$ for the large momentum $k_x\simeq k_{\mathrm{F}}$, which means that the amount of non-adiabaticity is maximized for the conduction electrons with $v_x^s\simeq v_{\mathrm{F}}$ because the traveling time through the spin spiral of these electrons, d/v_x, is much shorter than the period of the precession of the spins of the conduction electrons around the exchange field J. In Ref.[4], Levy and Zhang approximate that $\cos(\phi/2)\to 1$ and $\sin(\phi/2)\to\tan(\phi/2)\to(k_x/k_{\mathrm{F}})\xi$. It should be noted that for a thin spin spiral where $\xi=l_J/d$ is comparable to or larger than unity, the estimation of the scattering rate $W_{\mathbf{k}\mathbf{k}'}^{ss'}$ in our theory for large momentum k_x is much smaller than that obtained by Levy and Zhang because the factor $\tan(\phi/2)$ in our calculation is always less than unity while the factor $(k_x/k_{\mathrm{F}})\xi$ used in Ref.[4] is larger than unity. Since the resistivity is high for a high scattering rate, the magnetoresistance obtained in our theory is much lower than that obtained by Levy and Zhang, as shown below.

To obtain the non-equilibrium distribution function $f^s(\mathbf{k})$ from the Boltzmann equation (3), we assume that $f^s(\mathbf{k})=(\partial f^{s(0)}(\mathbf{k})/\partial\varepsilon)g^s(\mathbf{k})\simeq-\delta(\varepsilon_{\mathrm{F}}-\varepsilon(\mathbf{k},s))g^s(\mathbf{k})$, where $f^{s(0)}(\mathbf{k})$ is the distribution function in equilibrium. Then, Eq. (3) is reduced to

$$\begin{aligned}-ev_x^s E=&-\frac{1}{\tau^s(k_x)}g^s(k_x)+\frac{m}{2\pi\hbar^3}\int_{-k_{\mathrm{F}}^s}^{k_{\mathrm{F}}^s}\mathrm{d}k_x'|V_{\mathbf{k}\mathbf{k}'}^{ss}|^2g^s(k_x')\\ &+\frac{m}{2\pi\hbar^3}\int_{-k_{\mathrm{F}}^{-s}}^{k_{\mathrm{F}}^{-s}}\mathrm{d}k_x'|V_{\mathbf{k}\mathbf{k}'}^{s-s}|^2g^{-s}(k_x'),\end{aligned} \tag{11}$$

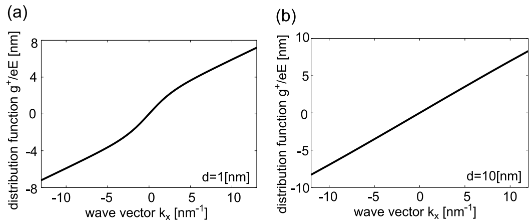

FIG. 1: The dependence of the distribution function, g^+/eE, on the momentum k_x for (a) $d=1$nm and (b) $d=10$nm, respectively.

where $k_{\rm F}^s$ is given by

$$k_{\rm F}^s = \sqrt{k_{\rm F}^2 + \left(\frac{\theta'}{2}\right)^2 + s\sqrt{(k_{\rm F}\theta')^2 + k_J^4}} \, . \tag{12}$$

The relaxation time $\tau^s(k_x)$ is given by $1/\tau^s(k_x) = 1/\tau^{ss}(k_x) + 1/\tau^{s-s}(k_x)$, where the spin-conserved relaxation time $\tau^{ss}(k_x)$ and the spin-flip relaxation time $\tau^{s-s}(k_x)$ are given by

$$\frac{1}{\tau^{ss'}(k_x)} = \frac{m}{2\pi\hbar^3}\int_{-k_{\rm F}^{s'}}^{k_{\rm F}^{s'}} {\rm d}k'_x |V_{\mathbf{kk}'}^{ss'}|^2. \tag{13}$$

The distribution function $f^s(\mathbf{k})$ is obtained by numerically solving Eq. (11)[17]. The resistivity of the spin spiral is calculated as $\rho = 1/(\sigma^+ + \sigma^-)$, where $\sigma^s = -(e/E)\int {\rm d}^3\mathbf{k}/(2\pi)^3 v_x^s f^s(\mathbf{k})$ is the conductivity of the spin-s electrons.

In the calculation of the scattering-in term, $\int {\rm d}^3\mathbf{k}'/(2\pi)^3[W_{\mathbf{kk}'}^{ss} f^s(\mathbf{k}') + W_{\mathbf{kk}'}^{s-s} f^{-s}(\mathbf{k}')]$, in Eq. (11), Levy and Zhang[4] assume that the non-equilibrium distribution function is proportional to the momentum k_x. However, we do not apply this diffusion approximation to the scattering-in term because we are interested in the resistivity for a spin spiral with $d < l_{\rm mfp}$. Figure 1 (a) and (b) show typical dependences of the distribution function obtained by Eq. (11), g^+/eE, on the momentum k_x for $d = 1$ nm and $d = 10$ nm, respectively, where the mean free path $l_{\rm mfp}$ is taken to be 5.9 nm. According to Fig. 1, we can verify that the diffusion approximation is not applicable to the region $d < l_{\rm mfp}$ while it is a good approximation to the region $d > l_{\rm mfp}$.

Before estimating the resistivity of a spin spiral, we should emphasize the validity of our calculation. The semi-classical Boltzmann equation is applicable when the system is larger than the width of the wave packet of the conduction electrons, i.e., the Fermi wavelength $\lambda_{\rm F}$. In our calculation, this condition equals $d > \lambda_{\rm F}$. For conventional ferromagnetic metals, the Fermi wavelength is on the order of a few angstrom, which is one order of magnitude smaller than l_J and $l_{\rm mfp}$[12]. It should also be noted that the derivative of the angle $\theta(x)$ is assumed to be constant in the derivation of the wave function (4). Thus, our calculation is valid for a spin spiral where the direction of the localized spin changes linearly in space.

Figure 2 shows the dependence of the MR ratio due to a spin spiral, defined by $(\rho - \rho^{(0)})/\rho^{(0)}$, on its period d. The values of the parameters we use are as follows. The Fermi energy $\varepsilon_{\rm F}$ and the sd-exchange coupling constant J are taken to be 5.0 eV and 0.5 eV, respectively. The Fermi wavelength $\lambda_{\rm F}$ is estimated to be 5.4 Å. The strengths of the impurity scattering, v and j, and the impurity concentration, $c_{\rm i}$, are estimated by the resistivity $\rho^{(0)}$ and the spin polarization β of a bulk ferromagnetic metal. The value of $\rho^{(0)}$ is taken to be 150 Ωnm, which is a typical value of the conventional ferromagnetic metals[18], while the value of β is taken to be from 0.3 to 0.9. Using these parameters, $l_J = \pi\hbar v_{\rm F}/(4J)$ is estimated to be 1.4 nm, and the mean free path $l_{\rm mfp} = (l_{\rm mfp}^+ + l_{\rm mfp}^-)/2$, where $l_{\rm mfp}^s = v_{\rm F}^s \tau^{s(0)}$, $v_{\rm F}^s = \hbar k_{\rm F}^{s(0)}/m$, $\tau^{s(0)} = \pi\hbar^3/[mc_{\rm i}(v - sj)^2 k_{\rm F}^{s(0)}]$, and $k_{\rm F}^{s(0)} = \sqrt{k_{\rm F}^2 + sk_J^2}$, is estimated to be 5.9 nm, which is approximately independent of the values of β.

As shown in Fig. 2, the MR ratio increases as the period d decreases. The higher the spin polarization of the bulk β is, the higher the MR ratio is. In the diffusive region $d > l_J, l_{\rm mfp}$, the MR ratio is estimated to be 1%-20%. On the other hand, for a thin spin spiral ($d \simeq 1-2$nm) with a high polarization ($\beta \simeq 0.8-0.9$), an MR ratio of more than 50% is predicted. Recently, a spin spiral of ferromagnetic Mn/W(001) with the rotation period $2d \simeq 2.2$ nm was created experimentally[19], whose period d is comparable to or smaller than l_J and $l_{\rm mfp}$. Thus, it is reasonable to consider such a sufficiently thin spin spiral $d < l_J, l_{\rm mfp}$. The values of the spin polarization β of the conventional ferromagnetic metals such as Fe, Co, Ni, and their alloys are about 0.5-0.7; for example, $\beta = 0.51$ for Co, 0.65 for $Co_{91}Fe_9$, and 0.73 for $Ni_{80}Fe_{20}$[20,21]. The value of β depends on the combination and the composition ratio of the ferromagnetic metals, and we can expect ferromagnetic metals with high spin polarizations. Thus, the prediction of our calculation for a spin spiral with high spin polarization β and a small period $d < l_J, l_{\rm mfp}$ will be confirmed experimentally.

The physics behind these results are as follows. The origin of MR due to a spin spiral is the mixing of the channels of the spin-up current and spin-down current due to the spin-dependent scattering potential $\hat{V}$. The channel mixing increases the scattering probability of the conduction electrons, and thus the resistivity. The mixing due to the scattering arises from the non-adiabaticity of the spins of the conduction electrons, which is characterized by $\tan[\phi(k_x)/2]$. In the limit of $d \to \infty$, the conduction electrons change the direction of their spins adiabatically, i.e., $\tan(\phi/2) \to 0$ for any momentum k_x, and the MR ratio tends to be zero. On the other hand, in the limit of $d \to 0$, the amount of non-adiabaticity that is maximized for the conduction electrons with large momentum k_x, i.e., $\tan(\phi/2) \to 1$ for $k_x \simeq k_{\rm F}$, and thus the MR ratio, increase as the period d decreases. In other words, the MR due to the spin spiral is mainly due to the conduction electrons with large momentum k_x. Since the MR arises from the asymmetry of the transport properties of

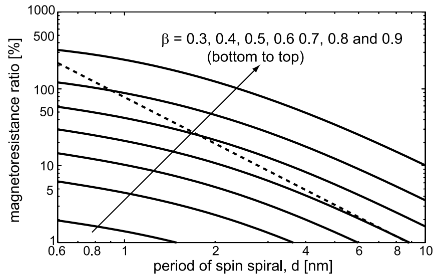

FIG. 2: The dependence of the magnetoresistance (MR) ratio of a spin spiral on its period d. The solid lines from bottom to top correspond to the MR ratio with the spin polarizations β=0.3, 0.4, 0.5, 0.6, 0.7, 0.8 and 0.9, respectively. The dashed line is the MR ratio estimated by the theory of Levy and Zhang[4] with $\beta = 0.5$.

the spin channels, the higher the spin polarization β is, the higher the MR ratio is.

The dashed line in Fig. 2 shows the MR ratio estimated by the theory of Levy and Zhang with $\beta = 0.5$[22];

$$\text{MR ratio} = \frac{4}{5}\xi^2 \left(\frac{\beta^2}{1-\beta^2}\right)\left(3 - \frac{5\sqrt{1-\beta^2}}{3}\right). \tag{14}$$

By comparing the solid line and the dashed line in Fig. 2, we find that the MR ratio in the diffusive region, $d > l_J, l_{\rm mfp}$, is proportional to $1/d^2$, as shown by Levy and Zhang[4]. On the other hand, in the ballistic region, $d < l_J, l_{\rm mfp}$, the MR ratio increases more slowly as the period d decreases compared to the diffusive region. It should be noted that the factor $\tan(\phi/2)$ is approximated to be $(k_x/k_{\rm F})\xi$ in Ref.[4], which is on the first order of $1/d$. However, for a thin spin spiral, the higher-order terms of $1/d$ also contribute to the calculations of resistivity, and the dependence of the MR ratio on the period d shifts from $1/d^2$. As shown in Fig. 2, the MR ratio obtained by our theory is much smaller than that obtained by Levy and Zhang. This is due to the fact that the estimated scattering rate by our calculation is much lower than that by Levy and Zhang, as mentioned above. The smaller the period d is, the larger the difference is in the amount of non-adiabaticity between our theory and that of Levy and Zhang, i.e., the difference in the values of $\tan(\phi/2)$ and $(k_x/k_{\rm F})\xi$. Thus, the difference in the MR ratio between our theory and theirs increases as the period d decreases.

In conclusion, we have studied the dependence of magnetoresistance due to a spin spiral on its period d by solving the Boltzmann equation. The scattering rate of the conduction electrons in the spin spiral is calculated by using the non-perturbative wave function of the conduction electrons, and the non-equilibrium distribution function is obtained by numerically solving the Boltzmann equation. An MR ratio of more than 50% is predicted for a thin spin spiral ($d \simeq 1 - 2$nm) with high spin polarization ($\beta \geq 0.8$). We also find that the MR ratio in the diffusive region is proportional to $1/d^2$, while in the ballistic region the MR ratio increases more slowly with decreasing d compared to the diffusive region.

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[22] The original paper of Levy and Zhang (Ref. 4) contains a typographic error in the coefficient of the second term on the right-hand side. In their paper, the coefficient is 5, not -5/3.